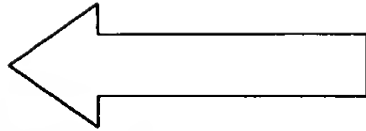
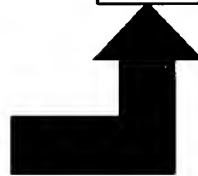
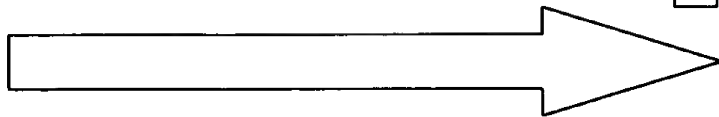


SCANNED, # 220



(1)



(6)



Fig. 1

Inventor(s): Dr. Stephen A. SCHUNK  
 Dr. John M. NEWSAM  
 DOCKET NO.: 078096/0105  
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# Performance Characteristics

Experimental Descriptors

<b>Synthesis</b> <ul style="list-style-type: none"> <li>• Reagents</li> <li>• Preparation Module</li> <li>• Conditions</li> <li>• Treatment</li> <li>• ...</li> </ul>	<b>Reactor</b> <ul style="list-style-type: none"> <li>• Types</li> <li>• Features</li> <li>• Catalyst Morphology</li> <li>• ...</li> </ul>	<b>Test</b> <ul style="list-style-type: none"> <li>• Reaction Conditions</li> <li>• Starting Material - Composition</li> <li>• ...</li> </ul>
-----------------------------------------------------------------------------------------------------------------------------------------------------------------------	--------------------------------------------------------------------------------------------------------------------------------------------	-----------------------------------------------------------------------------------------------------------------------------------------------



**Performance Characteristics**

**First Order Catalyst Characteristics**

- Crystallinity
- Defect Structures
- Particle Size Distribution
- ...



**Second Order Catalyst Characteristics**

- Redox Properties
- BET
- Heat of Adsorption
- Acidity
- ...

**Fig. 2**

Initial Substance  
Library

Operator

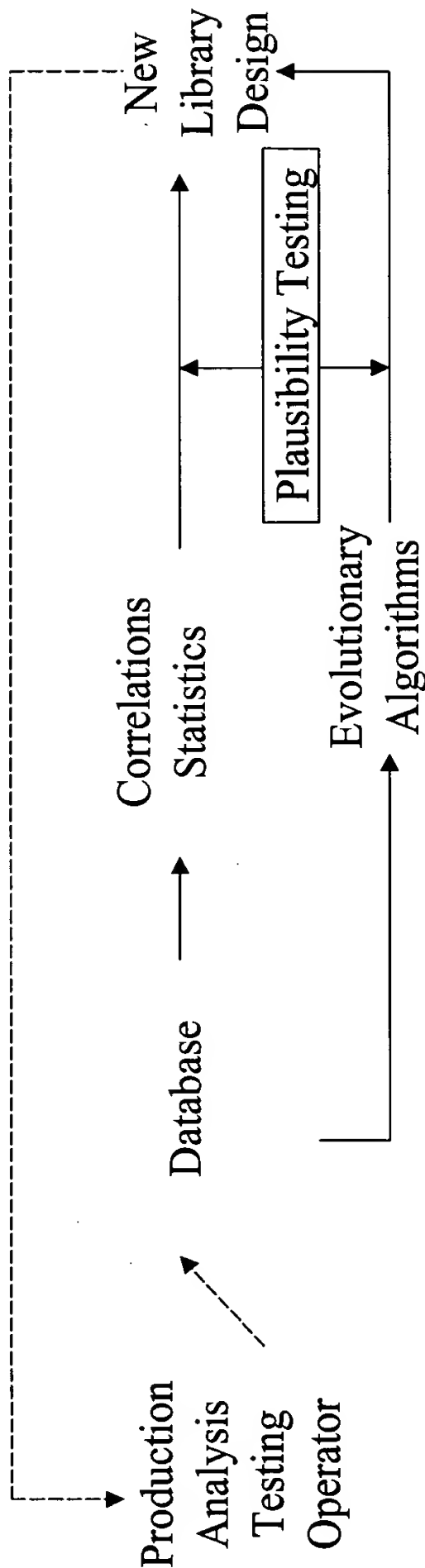
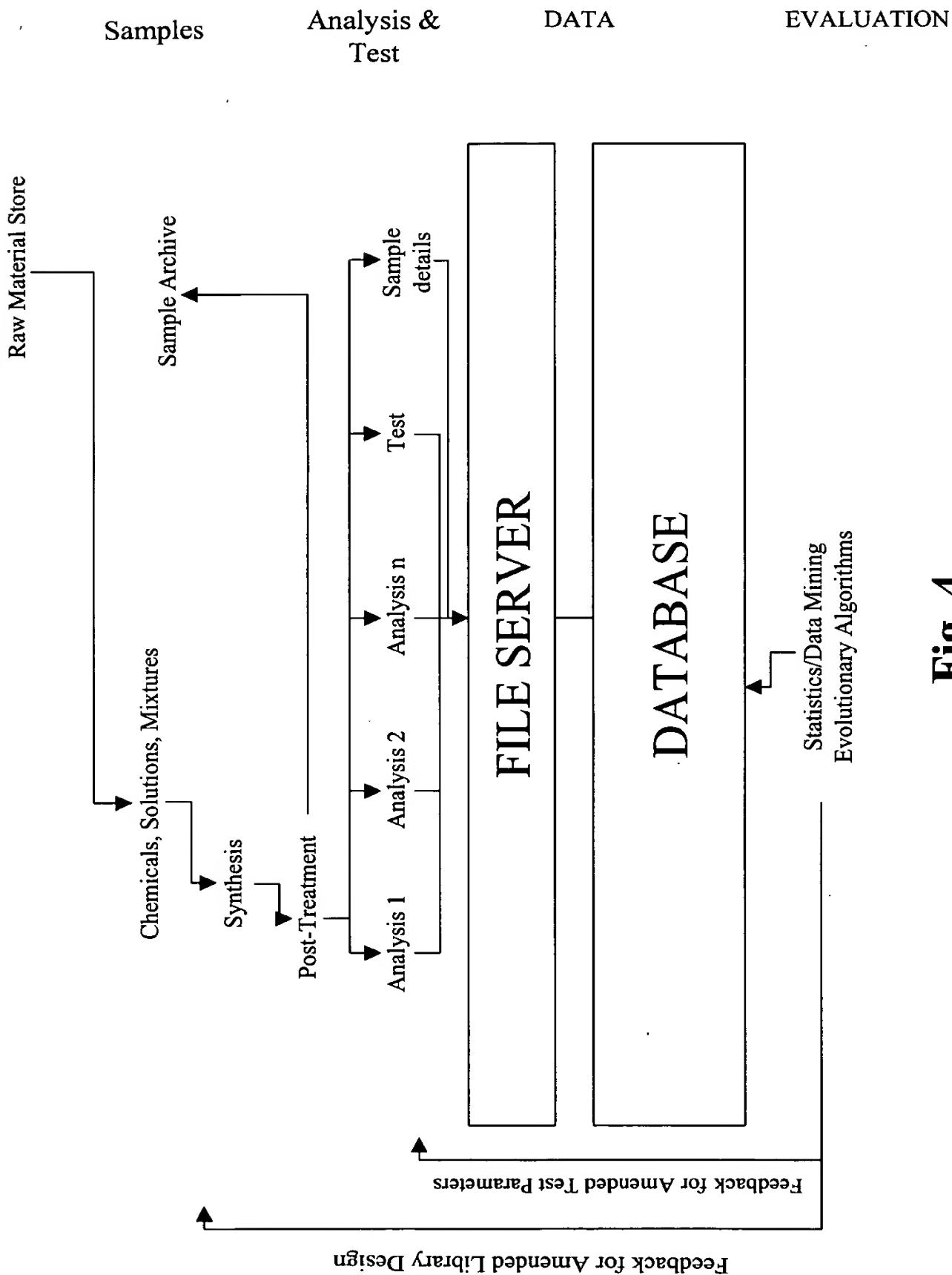


Fig. 3

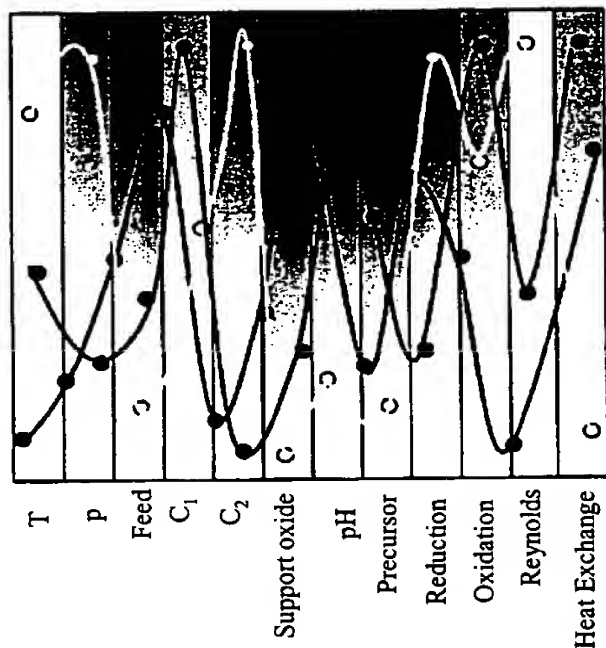
## Data Flow and Material Flow



**Fig. 4**

# Original Library Design and Tests Using the Entire Parameter Space

Step 1: Design of Library, Test  
and Process Conditions



Step 2: Data Acquisition

	Experiment 1	Experiment 2	Experiment n
T	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
P	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>
Feed	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>
C <sub>1</sub>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>
C <sub>2</sub>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>
Support oxide	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>
pH	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>
Precursor	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>
Reduction	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
Oxidation	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
Reynolds	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
Heat Exchange	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>

Activity	++	+	++
Selectivity	+	++	-

Fig. 5a

# Regression Analysis, Energies of the Parameter Space

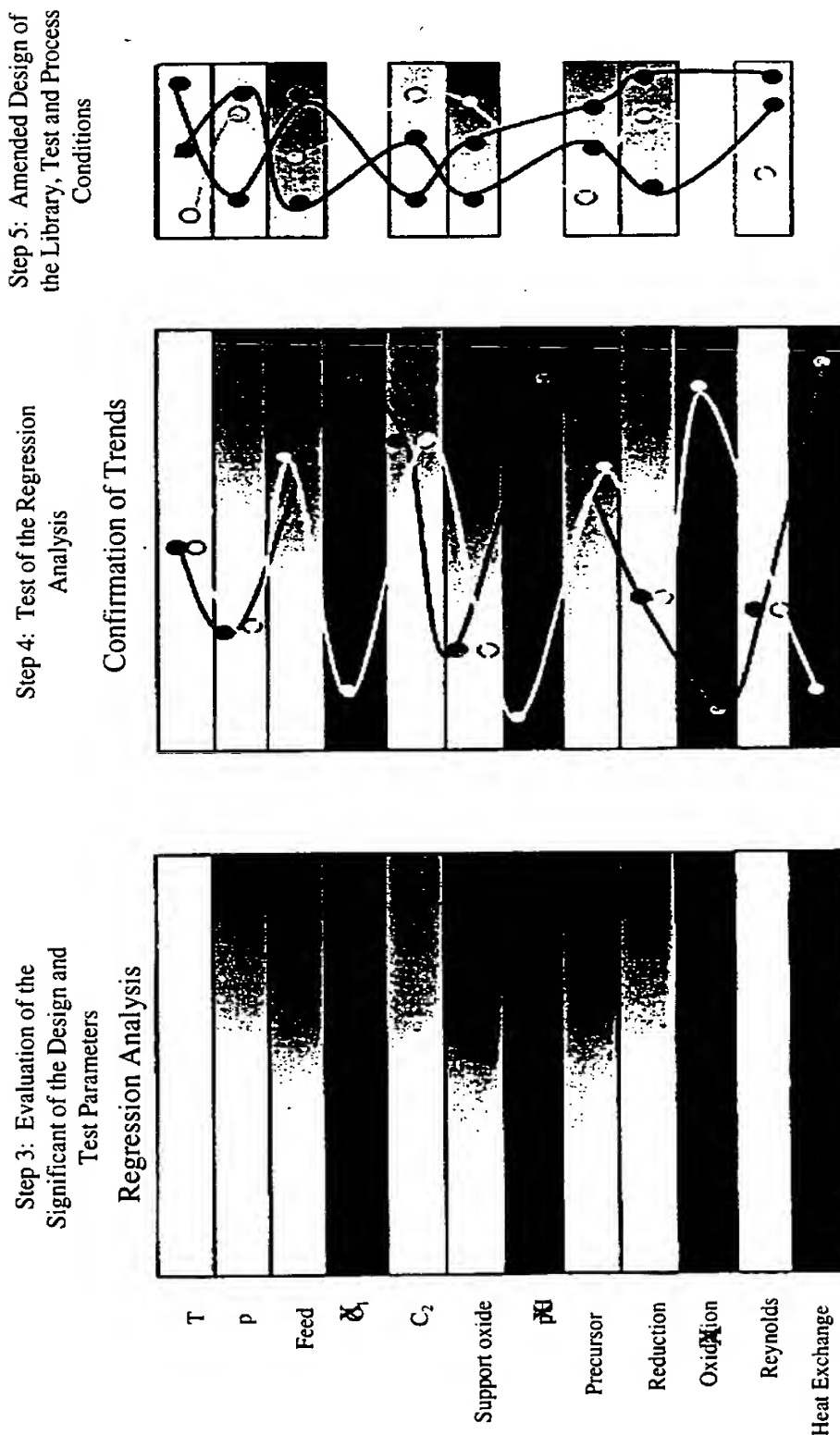


Fig. 5b

# Principle of Genetic Algorithms

Title: COMPUTER-AIDED OPTIMIZATION OF SUBSTANCE LIBRARIES  
 Inventor(s): Dr. Stephen A. SCHUNK  
 Dr. John M. NEWSAM  
 DOCKET NO.: 078096/0105  
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 RPEET/TJBURNS

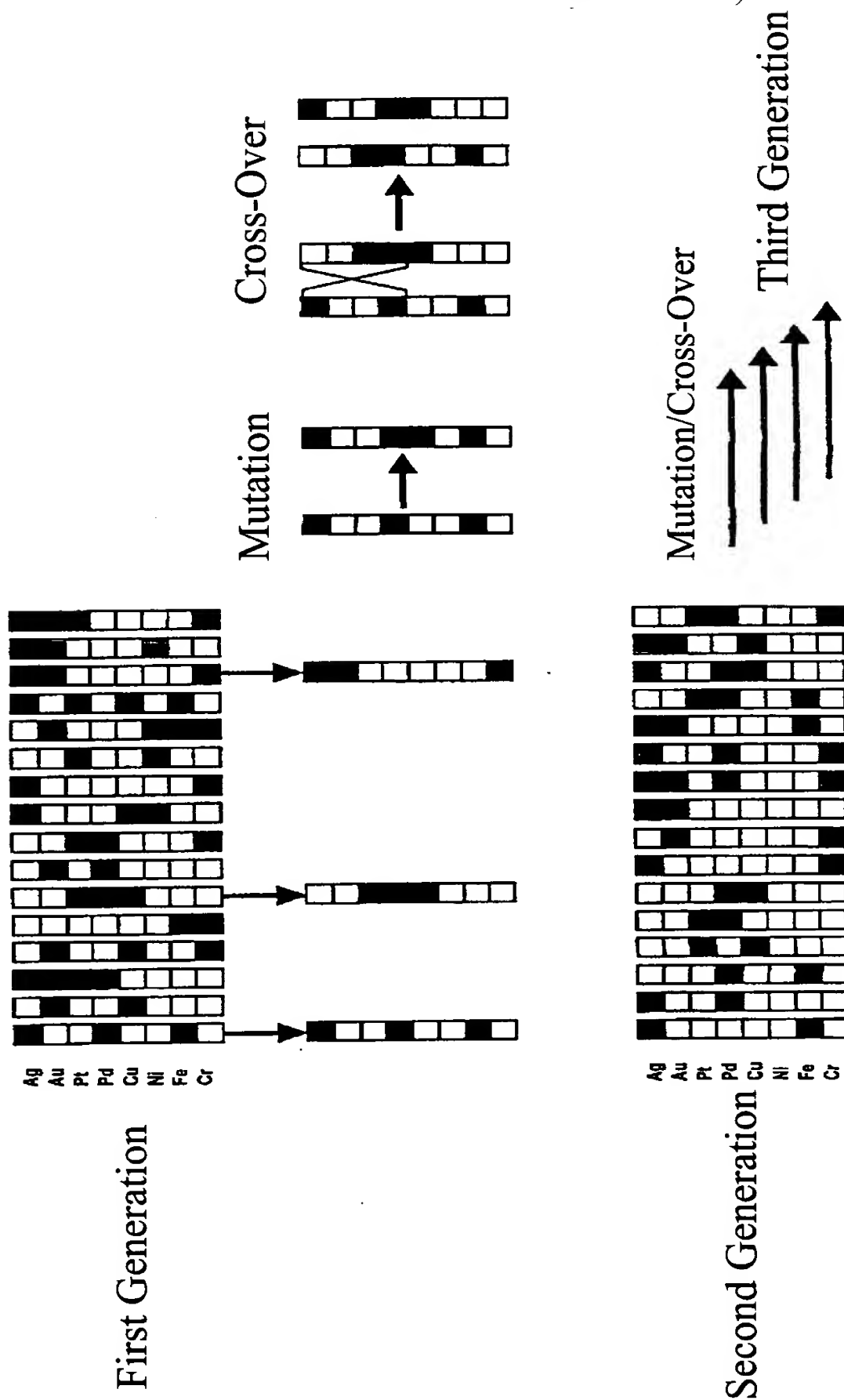


Fig. 5c

# Sensitivity Analysis of the Parameters of the Initial Library Pareto Diagram

Pareto Chart of Standardized Effects; Variable: U\_NOX  
7 factors, 5 Blocks, 96 Runs; MS Residual=128,2875

DV: U\_NOX

p=.05

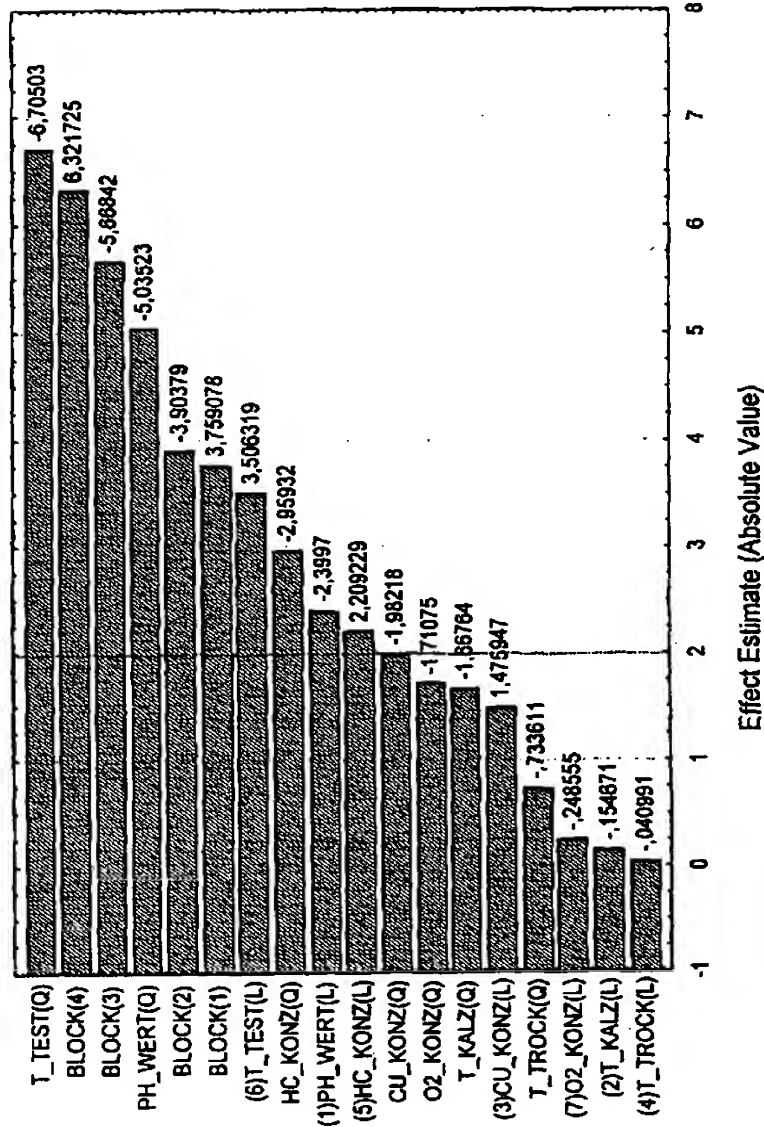


Fig. 6



# Sensitivity Analysis of the Parameters of the 1st Optimized Library Pareto Diagram

Pareto Chart of Standardized Effects; Variable: U\_NOX  
4 factors, 2 Blocks, 48 Runs; MS Residual=99,09295  
DV: U\_NOX

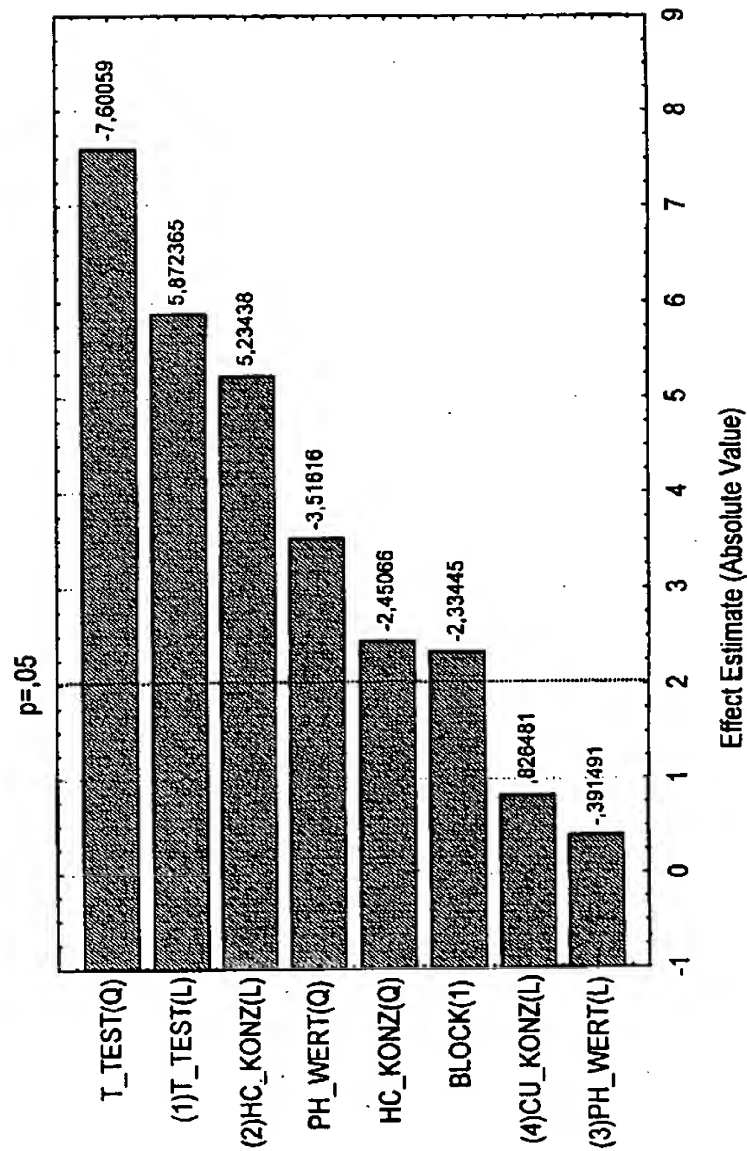


Fig. 7